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Developing Correlations for Prediction of Petroleum Fraction Properties Using Genetic Algorithms

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Résumé — Développement de corrélations pour la prédiction des propriétés des fractions pétrolières par les algorithmes génétiques — Notre étude concerne la caractérisation des fractions pétrolières dont les propriétés thermodynamiques et physiques peuvent seulement être connues par une expérimentation lourde et coûteuse due à la multiplicité de leurs constituants. Après une introduction des éléments et des nouvelles tendances dans l'utilisation des techniques d'intelligence artificielle, cet article prouve que les algorithmes génétiques peuvent être appliqués à ce domaine du pétrole. Par conséquent, nous proposons une approche empirique pour estimer les propriétés critiques et le facteur acentrique des fractions pétrolières, basée sur leurs points d'ébullition et densité facilement accessibles. Les algorithmes génétiques nous fournissent aussi une forme appropriée de fonction pour la prédiction de ces propriétés. Des résultats très prometteurs sont obtenus et plusieurs perspectives méritant d'autres investigations sont soulignées.

Abstract — Developing Correlations for Prediction of Petroleum Fraction Properties Using Genetic Algorithms — This paper deals with the characterization of petroleum fractions whose thermo-physical behaviours can only be known through expensive measurement efforts due to the multiplicity of their constituents. After introducing the issue and new trends in the use of artificial intelligence techniques, this paper shows how genetic algorithms can be applied to this field. Hence, we propose an empirical approach for estimating petroleum fractions critical properties and acentric factor based on their boiling point and density that can be easily obtained. Genetic algorithms provide us with a proper function form for the prediction. Moreover, very promising results are obtained and several relevant issues that deserve further investigations are emphasized.

NOTATIONS

P_c Critical pressure (bar)
SG Specific gravity
T_b Normal boiling temperature (K)
T_c Critical temperature (K)
V_c Critical molar volume (cm^3/gmol)
ω Acentric factor

INTRODUCTION

No matter how well advanced the knowledge is in the field of chemical analysis and in the property-structure relationships, an empirical approach based on correlation for estimating properties of oil fractions remains unavoidable because they are complex mixtures. This paper deals with the empirical determination of the most significant properties of liquids which are the acentric factor and the critical properties, namely, the critical pressure, the critical temperature and the critical volume. The reasons for the need to predict critical properties and acentric factor of petroleum fractions are widely known. Let us just briefly recall that the rationalization of energy use depends strongly on an accurate thermo-physical property prediction and that almost all fluid properties are related to the critical properties and the acentric factor.

The experimental estimation of these parameters requires sophisticated and expensive equipments as well as long and precise manipulations. Moreover, it is limited to substances with low molecular masses and that are stable near the critical points. The measurement of these characteristics for substances with high molecular mass becomes indeed difficult and gives uncertain results due to the thermal decomposition and the appearance of certain reactions around the critical points of the substances. In order to overcome this difficulty, correlations based approaches are widely used in the oil field. In other words, since the well-known group contribution methods cannot be used for the mixture of indefinite structures such as petroleum fractions, then the different correlation methods try to relate critical properties with other properties that are easily obtained through experiments such as the normal boiling point for instance.

Hence, over the years, several correlations have been proposed for the characterization of petroleum fractions. Simmrock *et al*. [1] surveyed 56 methods for estimating critical temperature, 55 for critical pressure and 54 for critical volume. Even if several accurate methods are reported, the characterization of the petroleum fractions still remains an active research area [2-11]. This is mainly due to the fact that a small error in critical property estimation can lead to a much higher error in thermo-physical property prediction, which can deteriorate the system operation efficiency. Therefore, improvements to the classical approaches by introducing new techniques are still necessary.

Artificial techniques brought a new sight to the characterization of petroleum fractions. To of the best of our knowledge, the pioneer of the use of these techniques is the work presented in [11], where authors proposed neural network for estimating normal boiling point and critical properties as well as acentric factor based on group contribution approach. Even if contribution group approach suffers from limited applications, encouraging results of this work motivated other authors to overcome this drawback. [12] introduced a neural network approach for the characterization of the petroleum fractions and studied the feasibility by comparing its results with those of the most known correlations. Other notable work is the one presented in [13]. This is based on a genetic algorithm which was used to optimize the values of the critical temperature and the critical pressure of a treated North Sea crude oil without the light fraction. As in the case of neural networks, genetic algorithms provide encouraging results and show that correlations can be improved by artificial intelligence techniques.

However, correlations still keeps the advantage of the easiness of use when one faces the lack of experimental data. For instance, the only way to benefit from results of [13] is to reproduce the same implementations and to redo the same computing and checking proceedings. From a practical point of view, the main reason of such a way of use of artificial intelligence techniques is that they avoid the difficult task of looking for a functional form when developing an empirical model [12]. The main motivation of our paper, which proposes reusable mathematical formulas based on genetic algorithms, is to benefit from the advantages of artificial intelligence techniques and correlations.

Proper functions require significant computational effort when they are nonlinear and involve large number of parameters. For this reason, genetic algorithms bring efficient solutions by avoiding local minima. Moreover, it improves the robustness toward the uncertainties on the correlation coefficients, due to their adaptive and stochastic aspects. Contrasting with the issue of petroleum fraction property prediction, genetic algorithms have been widely applied in several domains, especially in system optimizations and in economical predictions [14, 15]. Our work shows the potential of applying genetic algorithms to the thermodynamic field. Using a data set of 109 different hydrocarbons, we obtain interesting correlations in a short computing-time. The attractive point of implementing genetic algorithm to find correlation parameters instead of a black box is to provide users with a function that they can apply. Besides, if it is necessary, the function can be adapted without changing the model structure.

The paper is organized as follows. Firstly, Section 1 gives a brief overview of genetic algorithms. In Section 2, the proposed method is presented through an example. In Section 3, the results of our method are then compared to the ones obtained from the most general and widely admitted methods

in the petroleum characterization field, in order to show that our proposed formulas are still appropriate for petroleum fractions.

1 GENETIC ALGORITHMS

Genetic algorithm is a particular class of evolutionary algorithms, which are adaptive search techniques for approximating solutions of optimization and prediction problems. They are based on a biological metaphor which simulates processes in natural systems that are necessary for evolution, specifically those that follow the principles first proposed by Charles Darwin of the survival of the fittest [16, 17]. As such, they represent an intelligent exploitation of a random search within a defined search space to solve a problem. A population of abstract representations (chromosomes) of solution candidates (individuals) for an optimisation problem evolves toward better solutions.

Traditionally, solutions are represented in binary systems as an array of bits, but different encodings are also possible, such as integer or real encodings. The evolution begins from a population of completely random individuals (initialization) and happens in generations. In each generation, the fitness of the whole population is evaluated. Multiple individuals are stochastically selected (selection) from the current population according to their fitness, and mutated (mutation) or recombined (crossover) to form a new population (reproduction). The latter is then used in the next iteration. The algorithm stops when a solution is found satisfying minimum criteria or when a fixed number of iterations is reached.

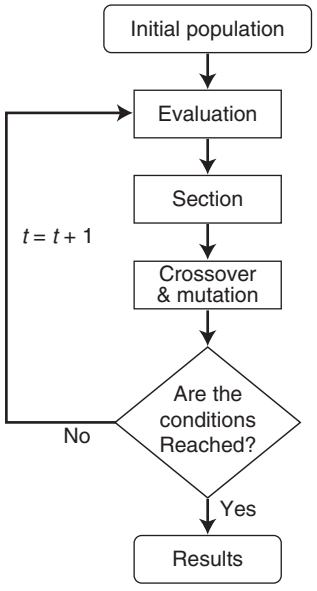

Figure 1
Genetic algorithm.

When applying genetic algorithm, one has to define at least a genetic representation of the solution domain (encoding) and at the same time a fitness function to evaluate the defined solution domain. In other words, one needs to fix the encoding of the solution as an array of bits, integers or floats in such a way that their parts are easily aligned due to their fixed size. Besides, at the encoding stage, one has to take into account the crossover and mutation operator complexity, which depends on the solution representation. Indeed, in some situations, in addition to problems associated with encoding and with evaluation definitions, one can face the problem of the definition of crossover and mutation operators in order to keep the validity of the solution. Furthermore, the fitness function has to be defined over the genetic representation in order to measure the quality of the represented solution. The fitness function is always problem dependent.

Once the genetic representation of the solution is known and the corresponding fitness function is defined, the genetic algorithm starts initializing a population of solutions randomly. Then the algorithm improves it by repetitive applications of crossover, mutation and selection operators *(Fig. 1)*.

After comparing real and binary encodings, we choose to represent the solution in our case as a binary array because it provides us with better results. The fitness is a sum of the square of the difference between the known value of the dealt property and the obtained one. Crossover and mutation operators are the uniform distribution [18] and the bit negation rule, respectively. The algorithm stops when the fitness value is less then the required precision. The following section gives more details about the used genetic algorithm, through an example of a given property.

2 APPROACH

The main *objective is to find a function that relate a critical property with the normal boiling point* (T_b) and the specific gravity (SG), from the following general function form:

$$\Pi_c = \left(aT_b^b + cSG^d + eT_b^f SG^g\right) \exp\left[\frac{SG+h}{T_b+i}\right] \qquad (1)$$

where $\prod_c$ is a critical parameter which can be T_c (in Kelvin), P_c (in bar), V_c (in cm^3/g.mol) or the acentric factor.

We can notice that:

– Equation 1 is very helpful for obtaining an order of magnitude about the values of different important parameters of the liquid considered. Only values of T_b and SG are needed, which are very easy to measure in a short time with inexpensive equipments.

– The polynomial equation combined with the exponential one is inspired from the literature. The final form is deduced after several tests of different combinations between polynomial and exponential functions of T_b and SG.
– Equation 1 is easy to compute: a more complicated equation than the one presented can discourage the user and a less complicated one does not provide us with good results.

We draw the reader's attention to the fact that the genetic algorithm is used to help us obtain the values of the constants *a-i* in Equation 1. In other words, the use of genetic algorithm leads us to propose an appropriate function form for each property. Since approaches to all critical parameters are the same, let us focus our attention to one critical parameter. Considering only the critical temperature (T_c), we have therefore to compute the constants of the following relation:

$$T_c = \left(aT_b^b + cSG^d + eT_b^f SG^g\right) \exp\left[\frac{SG+h}{T_b+i}\right] \quad (2)$$

One can note that the solutions we have to encode are the values of the constants in Equation 2. Using known experimental data, we firstly fix an interval of variation for each constant x_i of the equation by means of a linear adjustment. For example, we obtain $-10 \le a \le 10$ and $0 \le f \le 20$. More generally, we have $x_{imin} \le x_i \le x_{imax}$. Then, each constant is encoded in an array of 32 bits. Hence, each solution is represented by an array of 288 binaries. However, before starting the encoding, we transform each float x_i (a proposed value of a constant in the equation) into an integer g_i as follows:

$$gi = \frac{x_i - x_{imin}}{x_{imax} - x_{imin}}\, g_{max} \quad (3)$$

where $0 \le g_i \le g_{max}$ and $g_{max} = 2^{32} - 1$.

For more details about the range of constants, see Table 1.

The selection operator of the proposed genetic algorithm is the well-known stochastic roulette wheel. This aims at giving preference to better individuals and granting them more chance to pass on their genes to the next generation. The crossover occurs by means of a comparison of binary individual bits in the string between two parents. The bits are swapped with a probability of 0.5. A stochastic mutation is implemented. The algorithm provides each constant of the function with a 1% chance to be modified. At each step of the algorithm, a random value is computed for each constant in order to decide whether or not it will mutate. A constant mutation means that one bit is chosen randomly and modified. The algorithm stops when the maximal absolute error of the best solution is lesser than or equal to the admitted value.

A set of 109 experimental data points of pure hydrocarbon components was used to identify the proposed model. For that purpose, we used the DIPPR's data banks [19] developed by the Institute of Chemical Engineering of the University of Pennsylvania, the data banks of the Thermodynamical Research Center of the University of Houston of Texas [20] and the API's data banks [21, 22]. Table 2 summarizes the hydrocarbon family, the range of carbon number and the number of data used in the evaluation process.

TABLE 2

Hydrocarbon family of data bank

Component type	Range	number of compounds
Alkanes	$C_6 - C_{30}$	40
Alkenes	$C_6 - C_{20}$	15
Alkynes	$C_6 - C_{20}$	9
Aromatics	$C_6 - C_{28}$	20
Naphthenes	$C_6 - C_{22}$	25

We can fix different error limitations (1%, 2%, 3%, 4%, ...). The user of the program has to do a compromise between the quality of the solution and the CPU time. We can obtain very satisfactory results in less than 1 minute. The worst case we faced was 10 minutes of running time. Moreover, we can stop the algorithm at any moment we want. Figure 3 gives the running time on a Pentium III against the precision and the population size. Table 3 shows the results we obtain when we fix the error to 1%.

TABLE 1

Range of admitted values for constants of Equation 1

	a		B		c		d		e		f		g		h		I	
	x_{imin}	x_{imax}	x_{imin}	x_{imax}	x_{imin}	x_{imax}	x_{imin}	x_{imax}	x_{imin}	x_{imax}	x_{imin}	x_{imax}	x_{imin}	x_{imax}	x_{imin}	x_{imax}	x_{imin}	x_{imax}
T_c	-10	10	-10	10	-10	10	-10	10	5	25	0	20	-5	15	-15	5	-500	500
P_c	-4.10^6	8.10^6	-10	10	-10	10	-10	10	-10	10	-10	10	-10	10	-10	10	-500	500
V_c	-10	10	-10	10	-10	10	-10	10	0	1000	-10	10	-10	10	-10	10	-500	500
ω	-10	10	0	20	-10	10	-10	10	-20	20	-10	10	-10	10	-15	5	-500	500

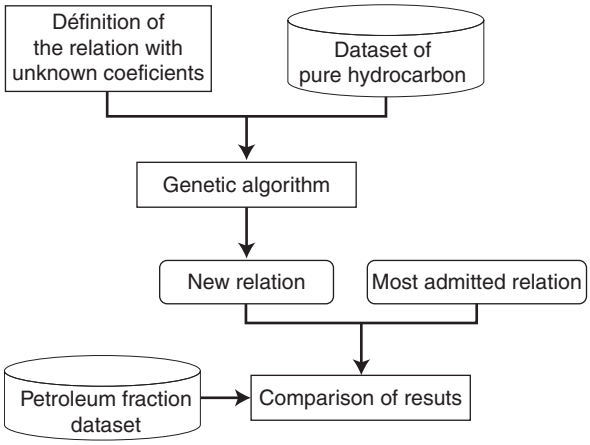

Figure 2

Proposed approach.

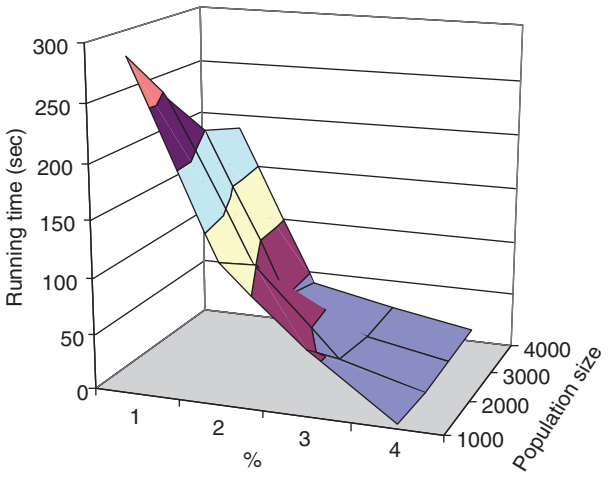

Figure 3

Genetic algorithm performance: critical temperature.

According to Equation 2, we obtain Table 3.

TABLE 3

Values of constants of Equation 2

a	b	c	d	e	f	g	h	i
0	0	0	0	17.8443	0.5965	0.2945	0	–100

From Table 3, Equation 2 can be rewritten as follows:

$$T_c = 17.8443 T_b^{0.5965} SG^{0.2945} \exp\left[\frac{SG}{T_b - 100}\right] \quad (4)$$

Figure 4 shows a comparison between results obtained from formula (4) and two most widely used correlations (Riazi-Daubert [23] and Lee-Kesler [24]) against experimental data. Each point corresponds to the percentage of the difference between an experimental critical temperature and the computed one. For readability reasons, an exponential trend curve is presented for each used formula. One can immediately observe that results of Equation 4 are the nearest to experimental values of critical temperature.

The same approach is applied to compute the other critical parameters and the acentric factor *(see Fig. 2)*. Table 4 gives the relations given by these parameters.

Table 5 summarizes precisions of functions (4-7) for pure hydrocarbons. It compares their precision with the best results of other correlations given in [23-26]. One can note from this table that the functions we are proposing give better results than those of other correlations for the data we have. Indeed, errors of the proposed formulas are noticeably lesser than the most used correlations.

In light of these encouraging results, we tested the reliability of the proposed functions by applying them to the petroleum fractions which are complex hydrocarbon mixtures. Hence, we use datasets of petroleum fractions and compare our obtained values with the ones computed by the most admitted relations.

TABLE 4

Obtained relations from genetic algorithm

Parameters	Relations	
Critical pressure	$P_c = 6.5243 \times 10^6 T_b^{-1.9781} SG^{1.8387} \exp\left[\frac{SG}{T_b - 250}\right]$	(5)
Critical molar volume[1]	$V_c = 0.0038\,(T_b - 273.16)^2 + 0.9814\,(T_b - 273.16)\,SG + 310.6783$	(6)
Acentric factor	$\omega = [0.0024 T_b - 0.8112 SG - 0.2347] \exp\left[\frac{SG}{T_b}\right]$	(7)

[1] For critical molar volume, we use $(T_b - 273.16)$ instead of T_b.

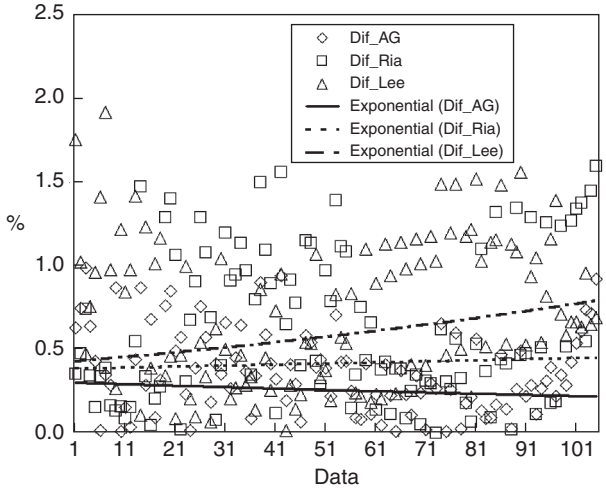

Figure 4

% of differences between computed and experimental critical temperatures results.

3 RESULTS

Let us recall that our objective is to provide mathematical proper functions that can be used for petroleum fractions having just boiling temperature and specific gravity properties. Hence, after obtaining these acceptable results for pure hydrocarbons *(see Table 5)*, relations (4-7) are then applied to oil fractions. For this application, we chose two Algerians crude oils for which we have 43 and 49 petroleum fractions, respectively. Distillation 'TBP' of these two oils provided us with interesting data, *i.e.* boiling temperature and specific gravity. These data are used for comparing the proposed functions, which are based on genetic algorithms, with those which are well-recommended in the literature. This aims at checking if relations obtained by means of genetic algorithms remain well-adapted to other data that we did not use for the computation of the proposed relations. Hence, in the following, we present differences between the results given by the genetic algorithm method and by the other ones for each property.

3.1 Critical Temperature

In order to compute the critical temperature, the relations using the boiling point and the specific gravity, which are well-recommended in the literature, are the ones of Riazi-Daubert [23] and of Lee-Kesler [24]:

$$T_c = 24.2787\ T_b^{0.58848}\ SG^{0.3596} \tag{8}$$

and

$$T_c = 341.7 + 811\ SG + \left(0.4244 + 0.1174\ SG\right)\ T_b + \left(0.4669 - 3.2623\ SG\right)\ \frac{10^5}{T_b} \tag{9}$$

respectively. T_c and T_b are expressed in °R.

The values of the difference between the previsions of our proposed model (4) and the ones of relations (8 and 9) for crude oils 1 and 2 are given in Figure 5 and Figure 6, respectively.

From Figure 5 and Figure 6 one can note that, for both crude oils, the results given by our suggested model are in perfect harmony (within 1% variations) with those given by the correlations proposed by Riazi-Daubert and Lee-Kesler. Hence our proposed model can be considered as a reliable one for this application.

3.2 Critical Pressure

As for critical temperature, we apply our model (5) as well as the Riazi-Daubert [23] and Lee-Kesler [24] ones to both crude oils for computing critical pressure. The Riazi-Daubert [23] and Lee-Kesler [24] models are respectively as follows:

$$P_c = 3.12281 \times 10^9\ T_b^{-2.3125}\ SG^{2.3201} \tag{10}$$

and

$$\ln(P_c) = 8.3634 - \frac{0.0566}{SG} - \left(0.24244 + \frac{2.2898}{SG} + \frac{0.11857}{SG^2}\right)10^{-3} T_b + \left(1.4685 + \frac{3.648}{SG} + \frac{0.47227}{SG^2}\right)10^{-7} T_b^2 - \left(0.42019 + \frac{1.6977}{SG^2}\right)10^{-10} T_b^3 \tag{11}$$

with T_b in °R and P_c in psia.

TABLE 5

Precision of functions for pure hydrocarbons

Parameters	Average absolute error (%)		Maximal error (%)		Minimal error (%)	
	Best other correlation	AG	Best other correlation	AG	Best other correlation	AG
T_c	0.6230	0.3500	1.5939	0.9674	0.0022	0.0006
P_c	5.0230	2.7225	10.4303	6.6039	1.2592	0.0677
V_c	2.0805	0.8063	4.0805	2.5523	0.9033	0.0099
ω	11.8461	9.9050	14.1317	16.8543	1.3810	0.1290

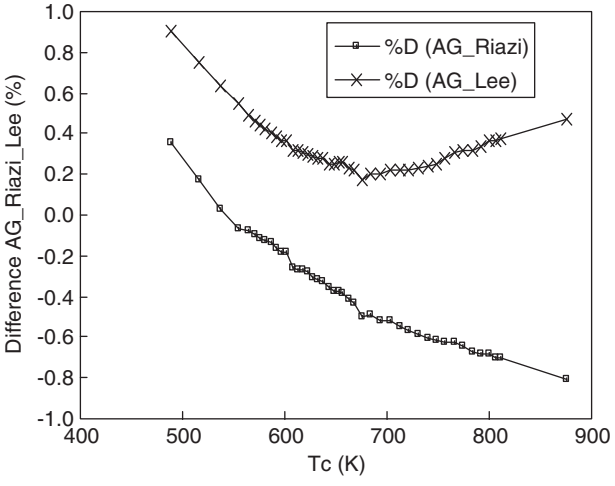

Figure 5

Crude oil 1: % of difference between genetic algorithm previsions and the ones of relations 8 and 9.

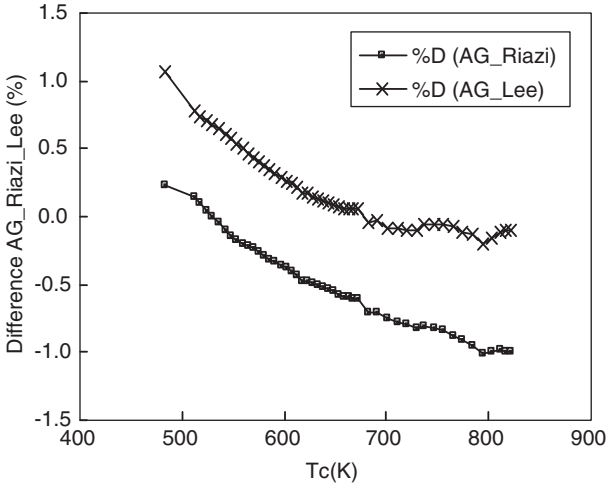

Figure 6

Crude oil 2: % of difference between genetic algorithm previsions and the ones of relations 8 and 9.

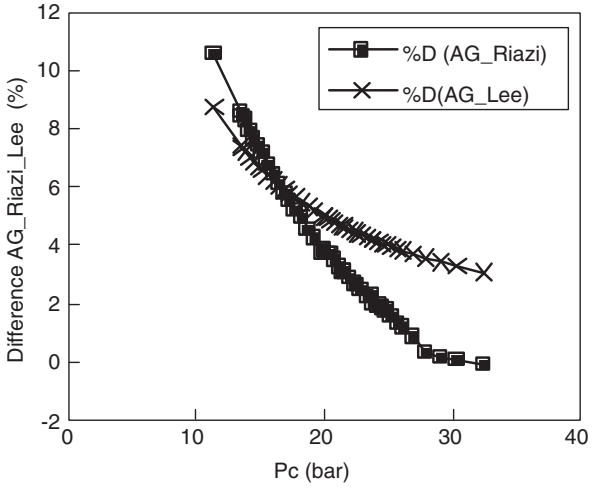

Figure 7

Crude oil 1: % of difference between genetic algorithm previsions and the ones of relations 10 and 11.

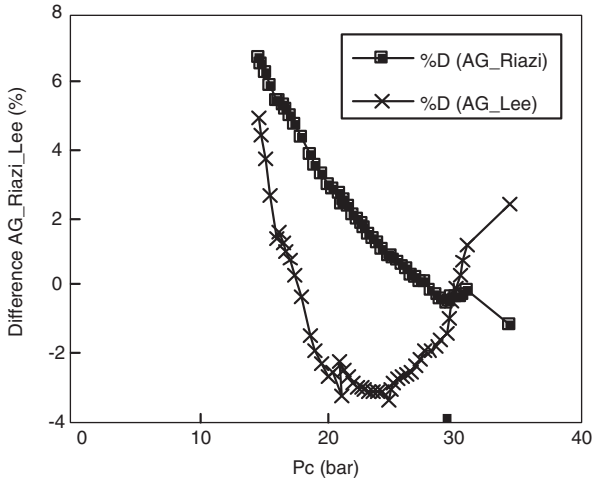

Figure 8

Crude oil 2: % of difference between genetic algorithm prevision and the ones of relations 10 and 11.

Figure 7 and Figure 8 show the difference between the prediction of our proposed model and of both other models for crude oils 1 and 2, respectively.

For critical pressure, the percentages of differences between the proposed model and the ones recommended by the literature are more significant than for critical temperature. However, the results are still encouraging: the percentage of difference exceeds only once 10% but remains less than 11% *(see Fig. 7)*.

3.3 Critical Molar Volume

The same comparisons are done. The functions taken into consideration are the Riazi-Daubert1 [23] and Riazi-Daubert2 [25] relations:

$$V_c = 7.5214 \times 10^{-3}\, T_b^{0.2896}\, SG^{-0.7666} \quad (12)$$

and

$$V_c = 6.233 \times 10^{-4}\, T_b^{0.7506}\, SG^{-1.2028} \exp [-1.4679 \times 10^{-3}\, T_b - 0.26404\, SG + 1.095 \times 10^{-3}\, T_b SG] \quad (13)$$

whith V_c in ft^3/lb and T_b in °R.

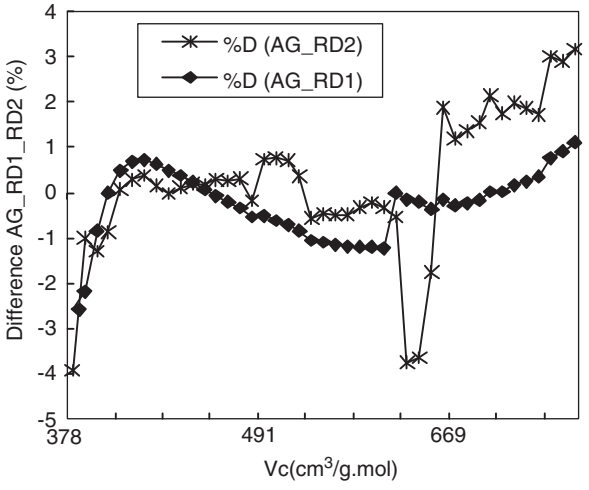

Figure 9

Crude oil 1: % of difference between genetic algorithm previsions and the ones of relations 12 and 13.

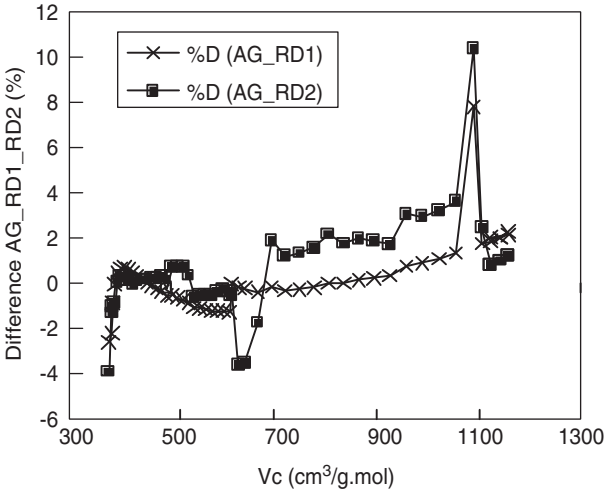

Figure 10

Crude oil 2: % of difference between genetic algorithm previsions and the ones of relations 12 and 13.

In Figure 10, one point exceeds 4% of absolute percentage of difference in prediction. Nevertheless, gathering all points of Figure 9 and Figure 10, the proposed model is satisfactory.

3.4 Acentric Factor

One can note from (7), that the acentric factor estimation does not depend on critical properties. However, this is not the case in the literature where the estimation of acentric factor requires an estimation of critical properties. Hence, to carryout the comparison, we use relations (8) and (9) to compute the critical temperature and relations (10) and (11) to compute the critical pressure. More precisely, the obtained values of acentric factor from model (7) are compared against two approaches: the first ones use both Riazi-Daubert relations for computing critical temperature and pressure and the second one uses both Lee-Kesler relations. Once the critical properties are computed, the following Edmister equation [26] is used to estimate the acentric factor:

$$\omega = \frac{3}{7}\left[\log \frac{P_c}{\frac{T_c}{T_b} - 1}\right] - 1 \qquad (14)$$

where P_c is the critical pressure in atmospheres.

One can note from Figure 11 and Figure 12 that the application of the literature based approaches gives us divergent results. At the same time, our proposed model can be considered as the one providing intermediate solutions. Besides, the absolute difference of acentric factor estimation for both oils does not exceed 10%. Hence, our model can be considered satisfactory for this thermophysical parameter.

CONCLUSION

In this paper, we present an approach based on genetic algorithm in order to propose a new function form for the prediction of critical properties of petroleum fractions as well as the acentric factor. In spite of the lack of data, we show that the functions we obtained provide us with values near those obtained from the most widely used functions in the literature. The proposed correlations can thus be applied to a wide range of temperatures and doe not require information about the oil compounds. It is obvious that, with more experimental data, the obtained functions can be improved with our proposed genetic algorithm. It is basically this fact that motivates us to present our results.

Several issues deserve further investigations. Improvement to the proposed functions is possible through parameters extension or adjustment using genetic algorithm. On the other hand, if experimental data are available, it is possible to use genetic algorithm to estimate the petroleum fraction compounds.

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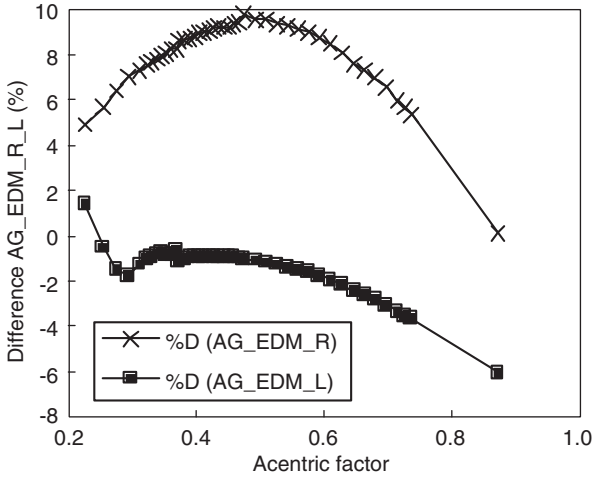

Figure 11

Crude oil 1: % of difference between genetic algorithm previsions and the literature based approach.

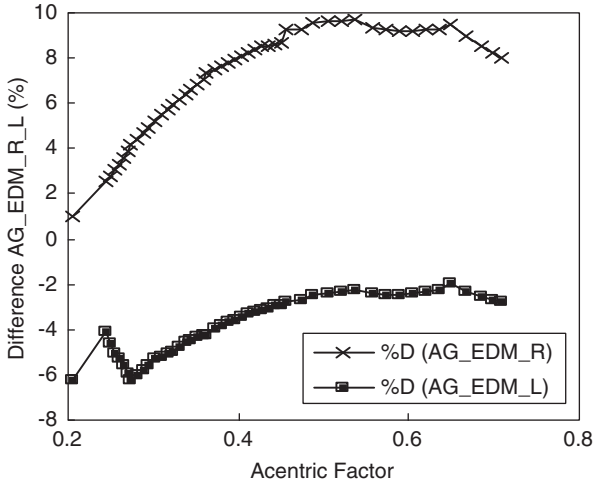

Figure 12

Crude oil 2: % of difference between genetic algorithm previsions and the literature based approach.

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